Argonne NATIONAL LABORATORY

An approach to discrete adjoints for MPI-parallelized C++ models applied to the NASA/JPL Ice Sheet System Model

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Argonne National Laboratory
NASA Jet Propulsion Laboratory

Feb/2014 TU Darmstadt, Germany

outline

- what this is for
- principles of AD
- changes in ISSM
- changes in Adol-C
- external solvers
- adjoinable MPI
- performance

Greenland

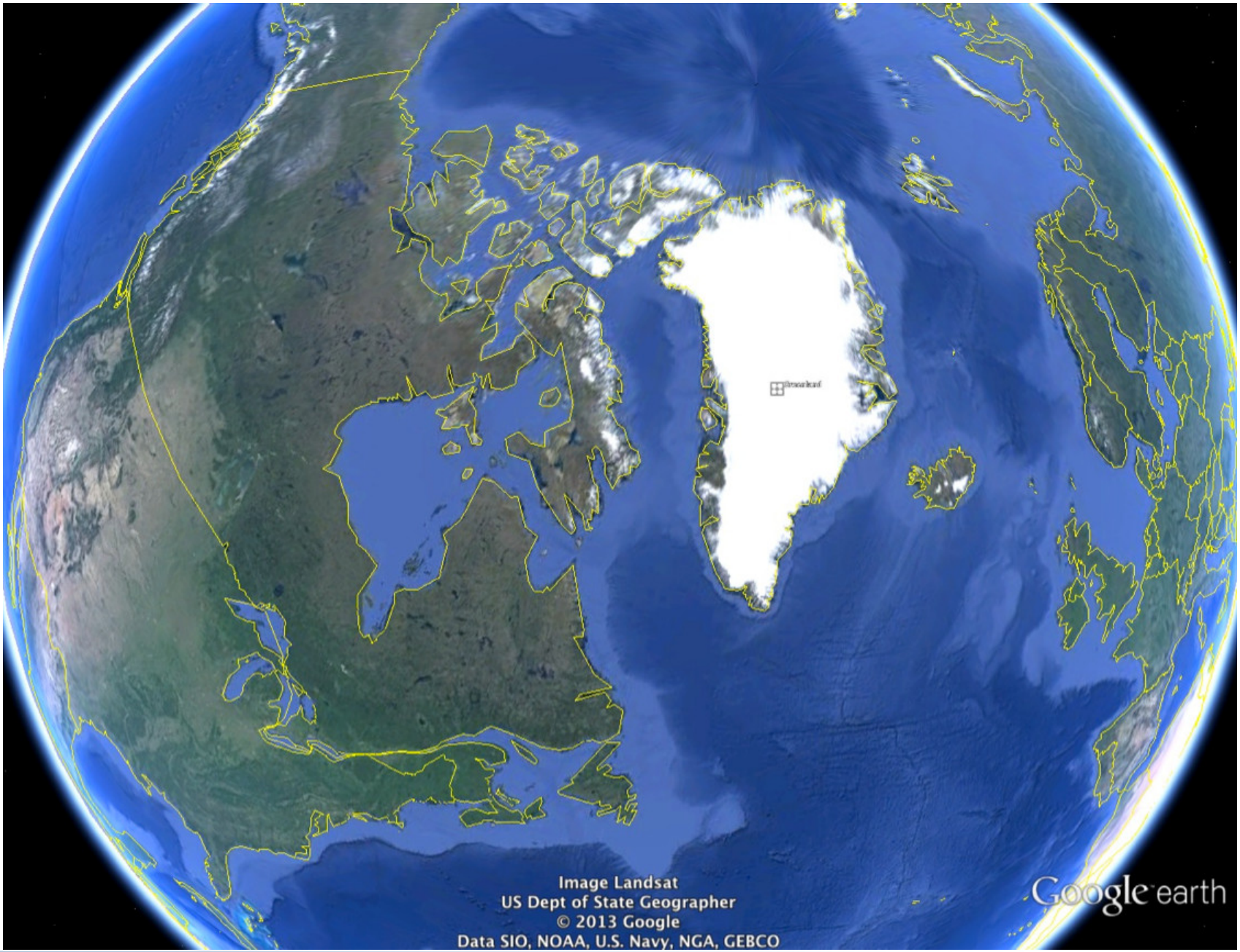
Image Landsat
US Dept of State Geographer
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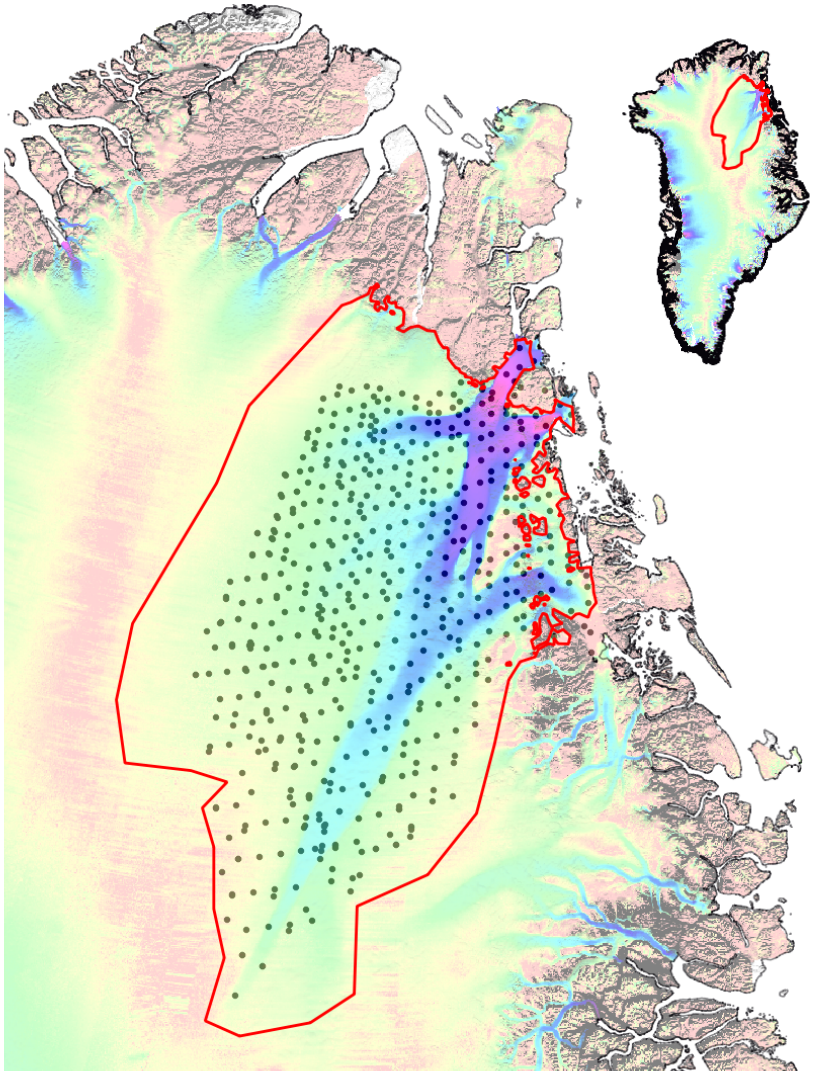
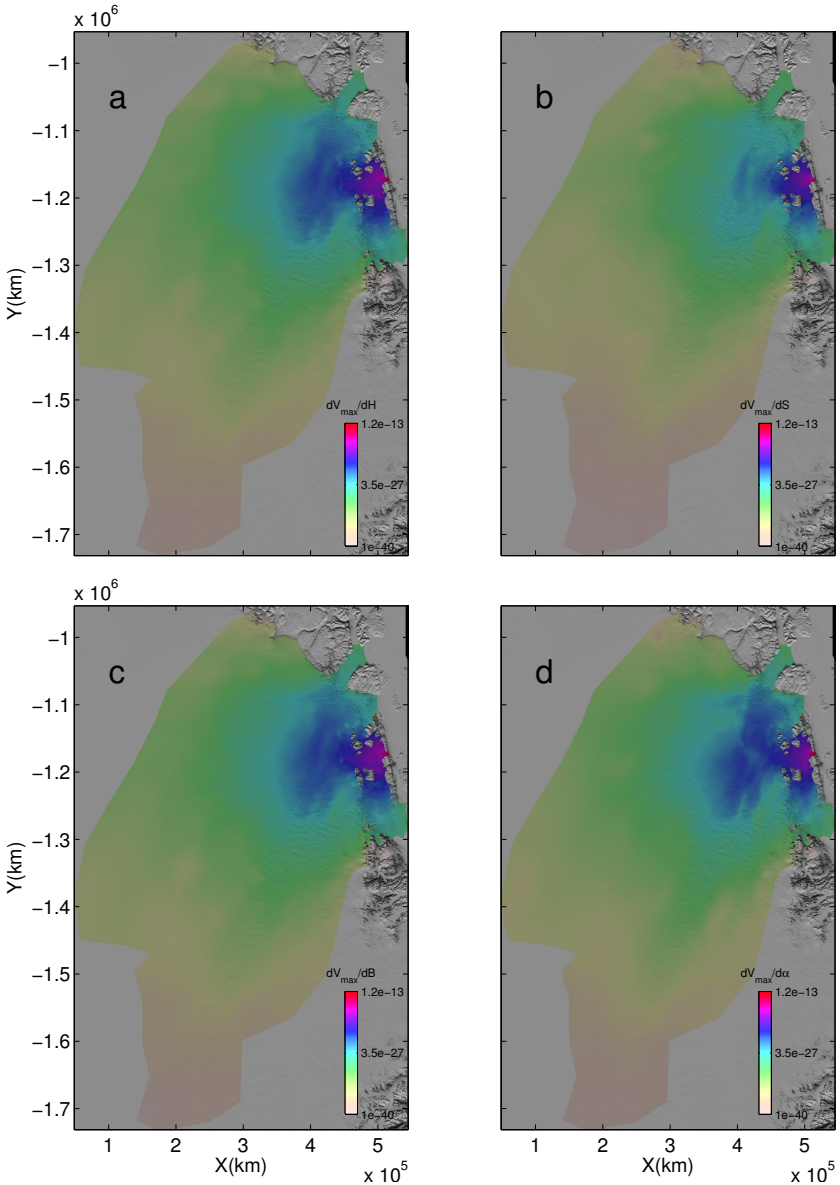
Data SIO, NOAA, U.S. Navy, NGA, GEBCO
Google earth

the North-Eastern Ice Stream on Greenland



- velocity field
- red boundary shows domain of interest
- dots indicate observation data
- surface observations by satellite/stations
- drilling holes is expensive
- goal is model tuning for prediction of sea level rise

sensitivity studies - maximal velocity with respect to



- a: H - ice thickness
- b: S - surface elevation
- c: B - bed elevation
- d: α - friction coefficient

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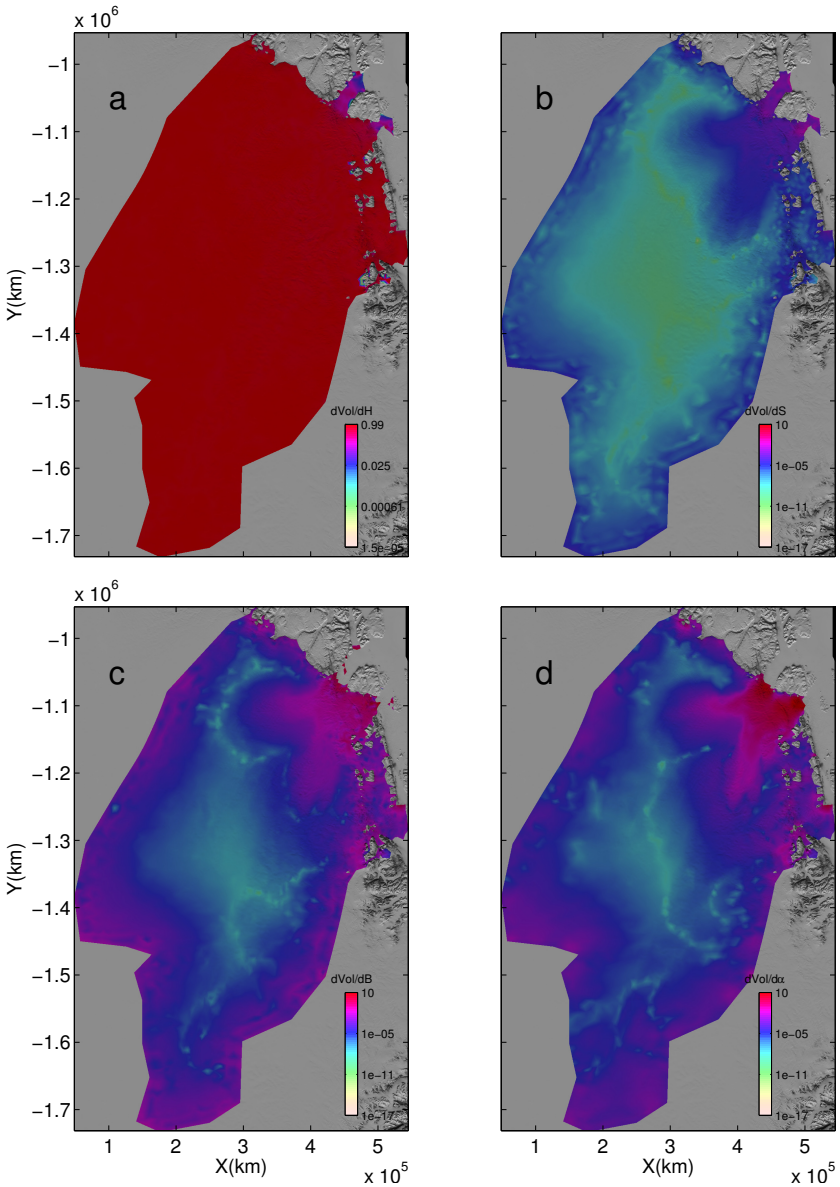

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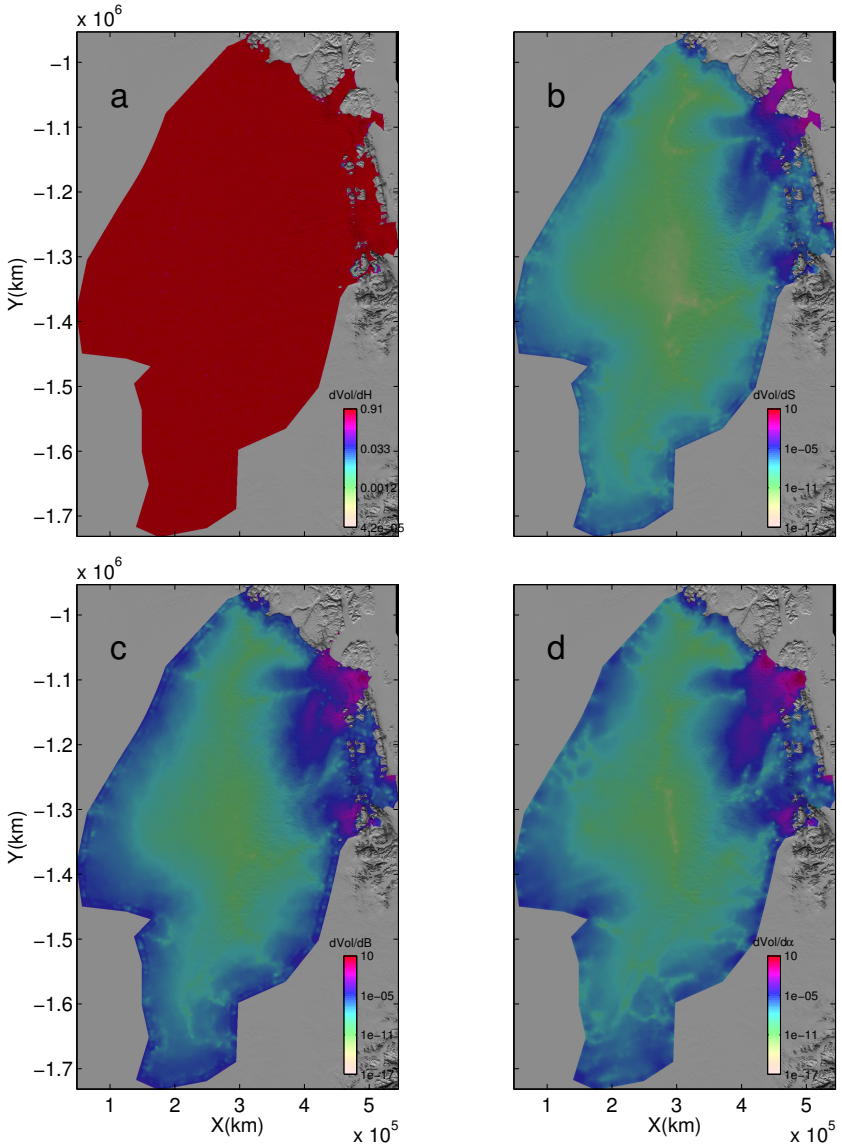
sensitivity studies (last week) - volume with respect to



- a: H - ice thickness
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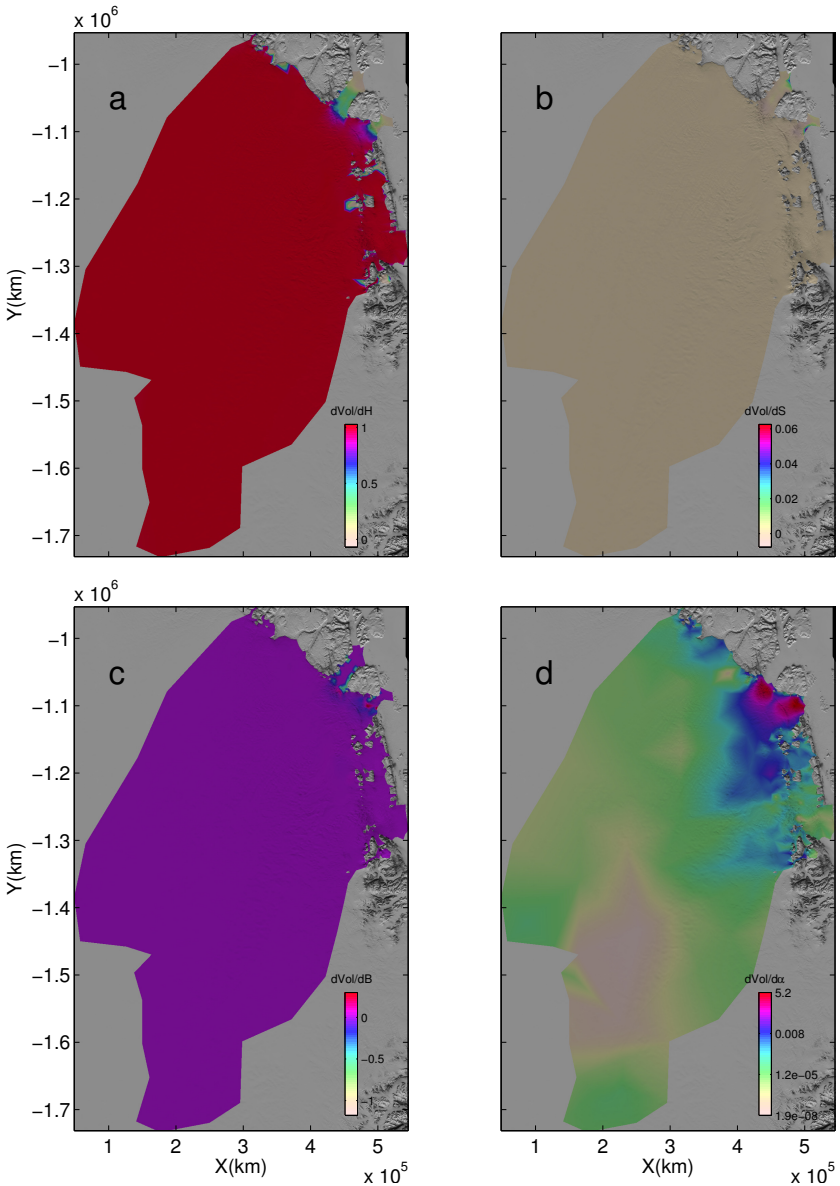
compared to earlier studies ran in higher resolution on Pleiades for longer model time

sensitivity studies - volume above floatation with respect to



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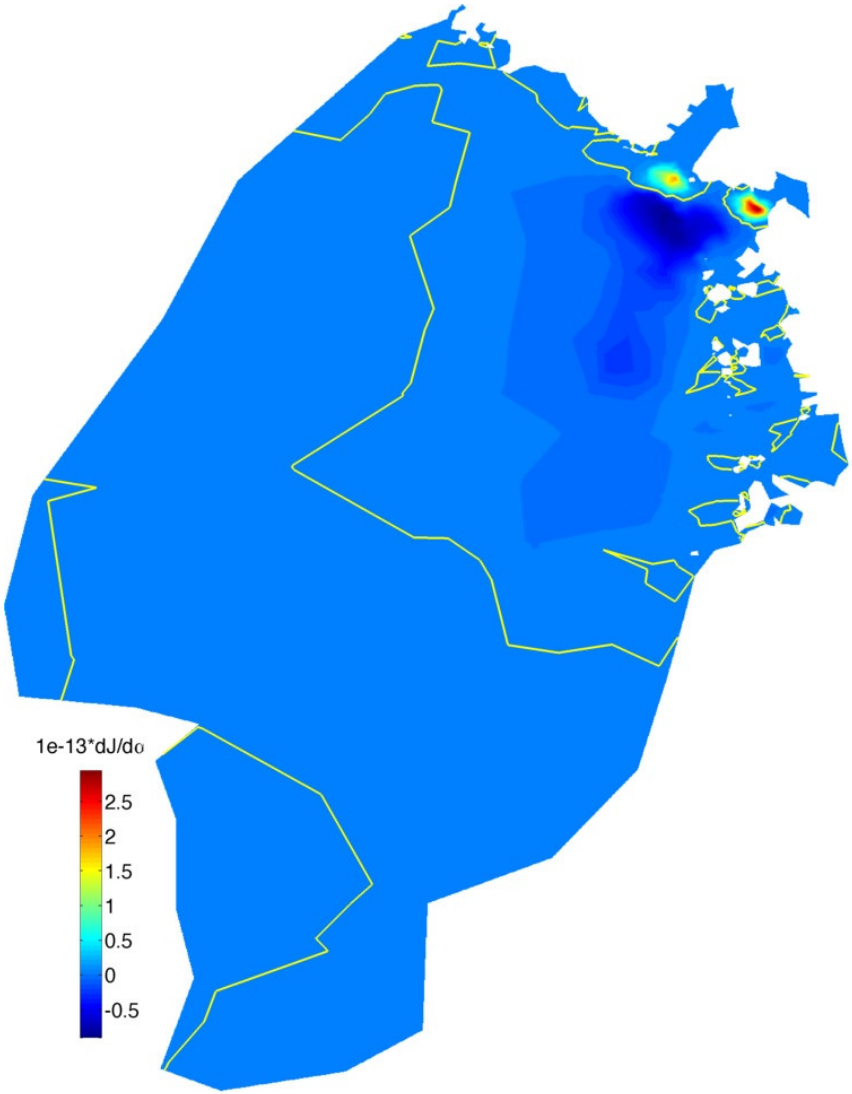
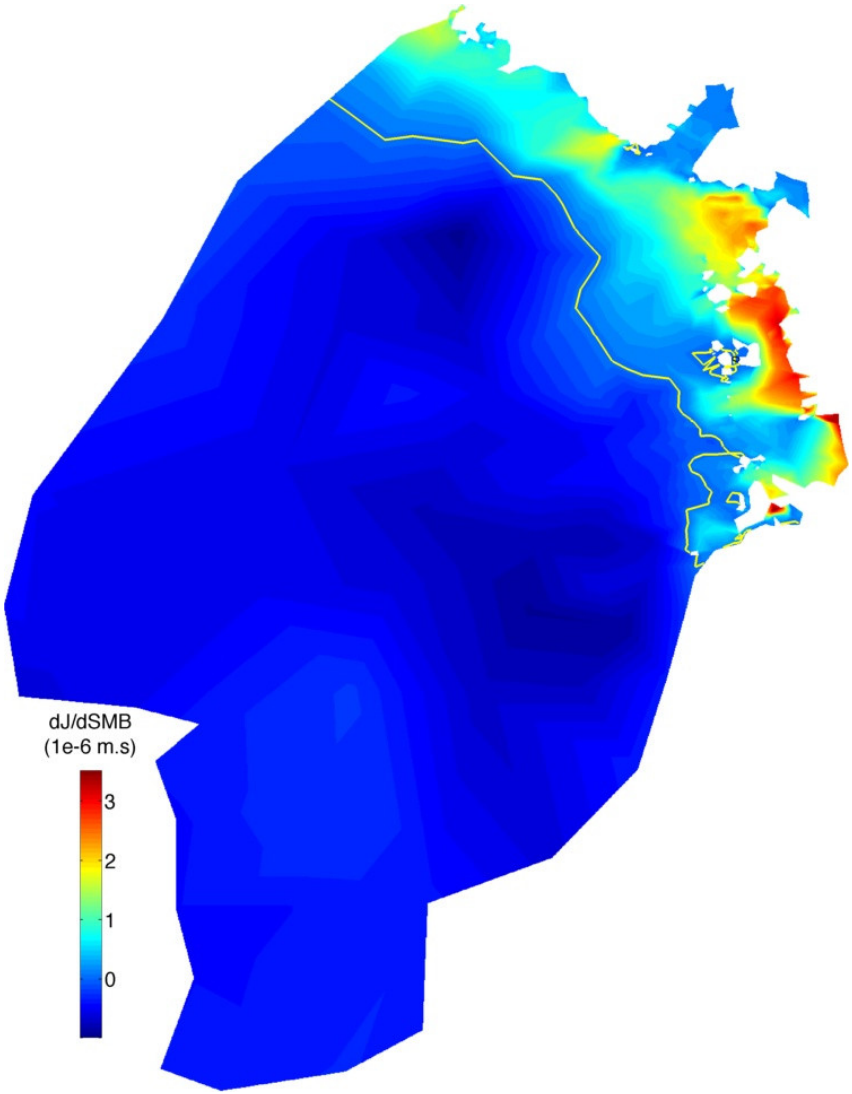
model-to-observation misfit of S to internal state



- with respect to friction coefficients
- L^2 integrated over time
- yellow lines indicate gradient sign switch
- part of an gradient $\rightarrow$ line search optimization loop

model-to-observation misfit of S to external boundary



- with respect to snow-mass-balance
- snow fall given as (external) reanalysis of climate model runs
- hints at less snow fall on the coast, more inland
- means to adapt reanalysis if one assumes the ice sheet model is "correct"

presented at AGU meeting

why algorithmic differentiation?

given: some numerical model $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) : \mathbb{R}^n \mapsto \mathbb{R}^m$
implemented as a (large / volatile) program

wanted: sensitivity analysis, optimization, parameter (state) estimation, higher-order approximation...

1. don't pretend we know nothing about the program
   (and take finite differences of an oracle)
2. get machine precision derivatives as $\boldsymbol{J}\dot{\boldsymbol{x}}$ or $\bar{\boldsymbol{y}}^T\boldsymbol{J}$ or ...
   (avoid approximation-versus-roundoff problem)
3. the reverse (aka adjoint) mode yields "cheap" gradients
4. if the program is large, so is the adjoint program, and
   so is the effort to do it manually ... easy to get wrong but hard to debug

$\Rightarrow$ use tools to do it **automatically!**

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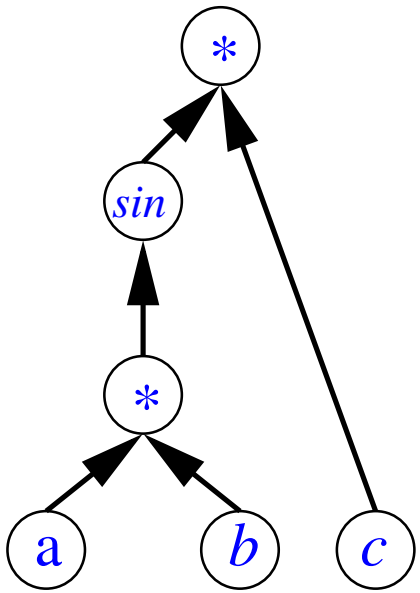
$\Rightarrow$ use tools to do it at least semi-automatically!

how does AD compute derivatives?

$f : y = sin(a * b) * c : \mathbb{R}^3 \mapsto \mathbb{R}$
yields a graph representing the order of computation:



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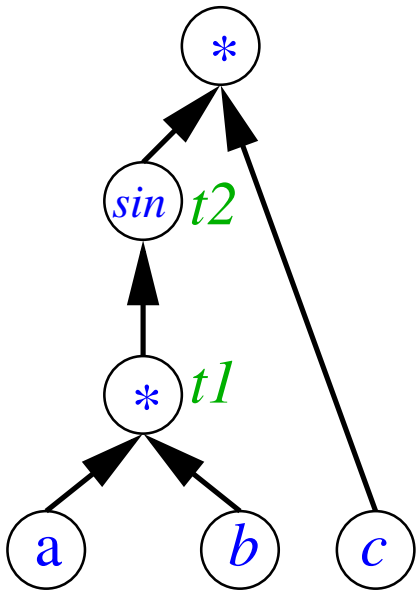

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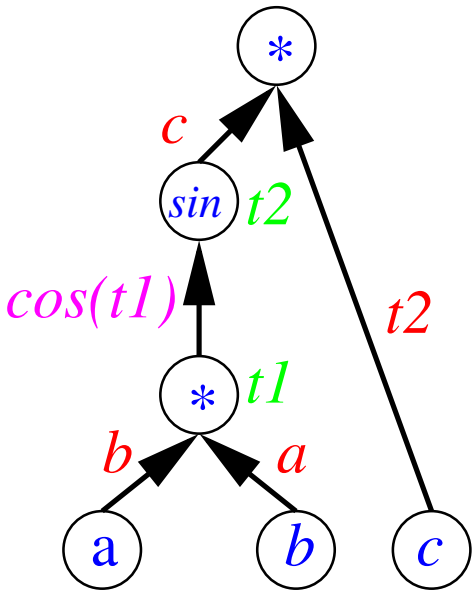

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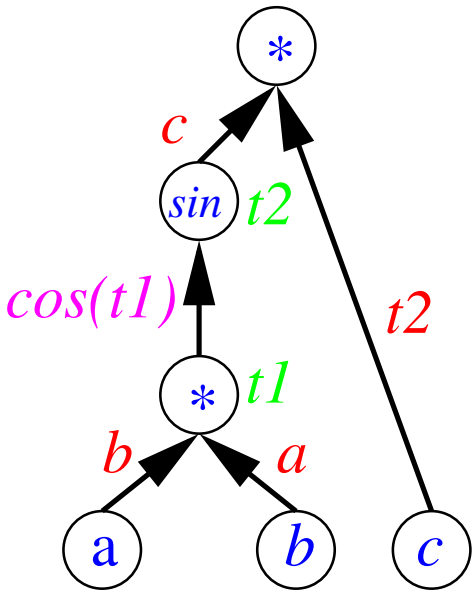

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What do we do with this?

forward mode with directional derivatives

- **associate** each variable v with a derivative $\dot{v}$
- take a point (a_0, b_0, c_0) and a direction $(\dot{a}, \dot{b}, \dot{c})$
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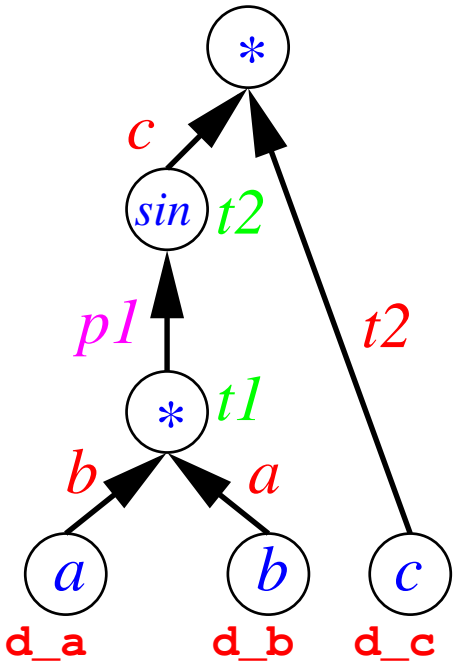

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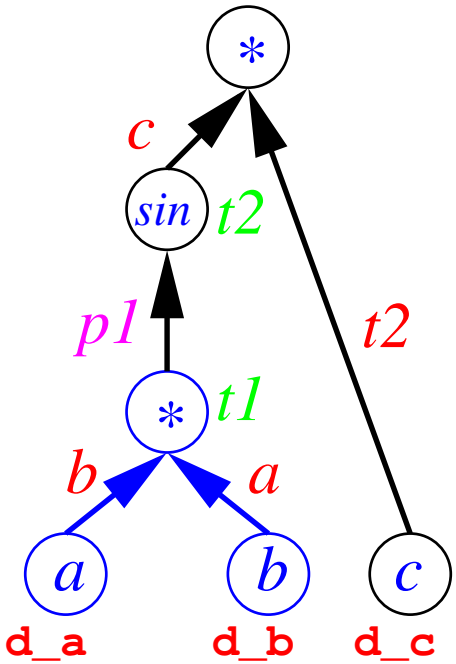

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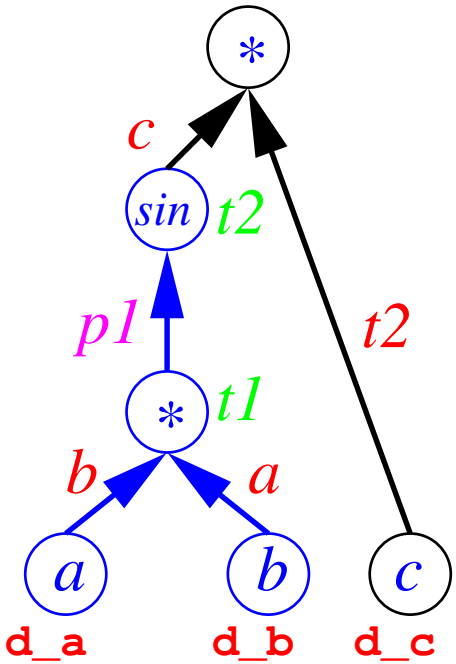

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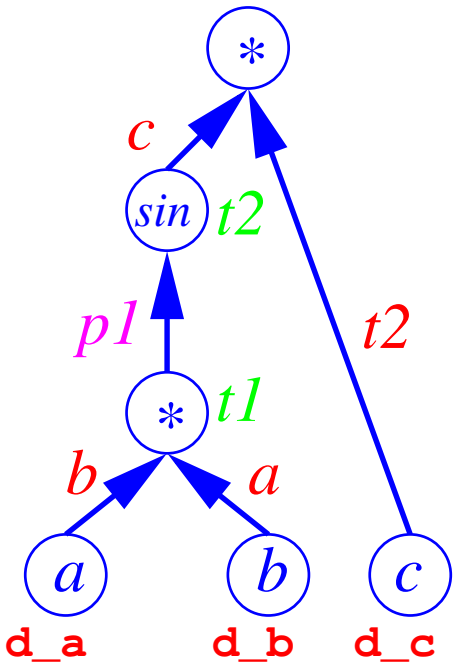

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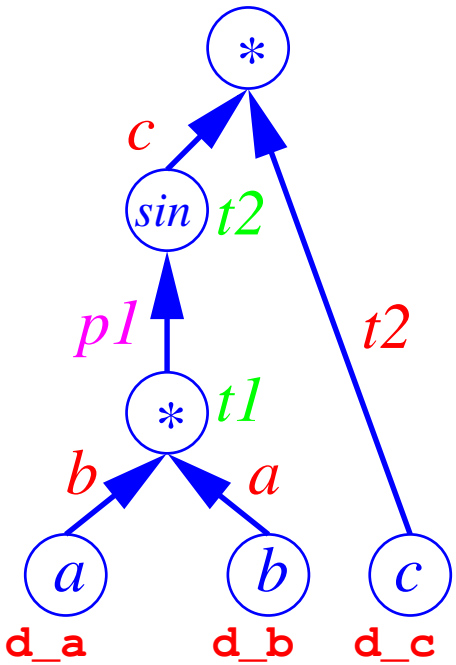

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What is in d_y ?

d_y contains a projection

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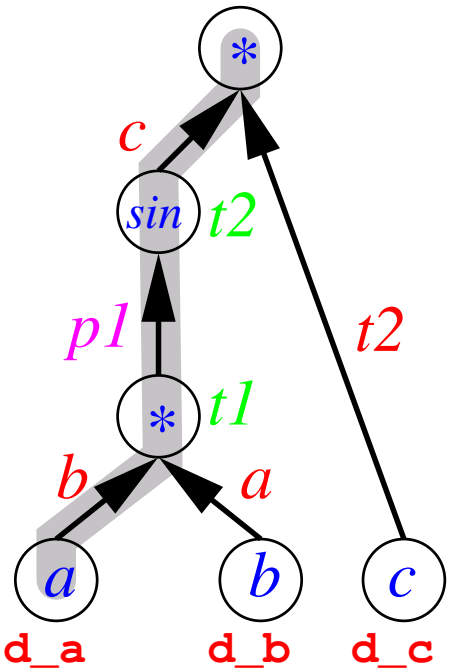

- yields the first element of the gradient
- all gradient elements cost $\mathcal{O}(n)$ function evaluations

sidebar: simple overloaded operators for a*b

in C++:

```
struct Afloat{float v; float d;};

Afloat operator *(Afloat a, Afloat b) {
  Afloat r; int i;
  r.v=a.v*b.v; // value
  r.d=a.d*b.v+a.v*b.d; // derivative
  return r;
};

// other argument combinations
```

in Fortran:

```
module ATypes
 public :: Areal
 type Areal
   sequence
   real :: v,d
 end type
end module ATypes

module Amult
  use ATypes
  interface operator(*)
    module procedure multArealAreal
    ! other argument combinations
  end interface
contains
  function multArealAreal(a,b) result(r)
    type(Areal),intent(in)::a,b
    type(Areal)::r
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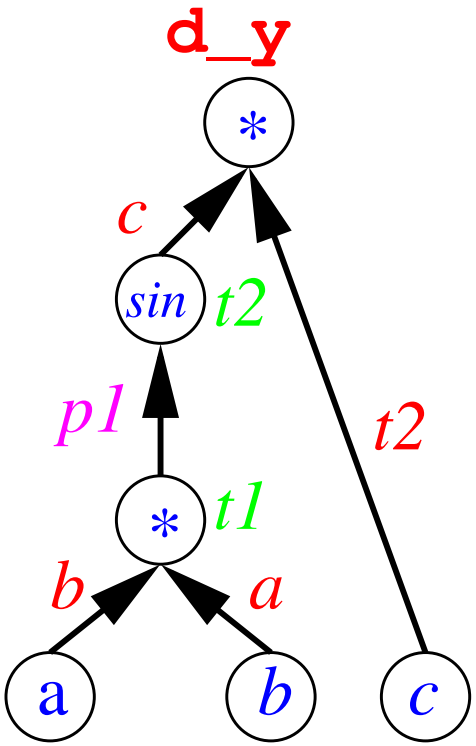
Operator Overloading $\Rightarrow$
A simple, relatively unintrusive way to augment semantics via a type change!

reverse mode with adjoints

- same association model
- take a point (a_0, b_0, c_0), compute y, pick a weight $\bar{y}$
- for each $v = \phi(w, u)$ propagate backward
  $\bar{w} += \frac{\partial \phi}{\partial w}\ \bar{v}; \quad \bar{u} += \frac{\partial \phi}{\partial u}\ \bar{v}; \quad \bar{v} = 0$



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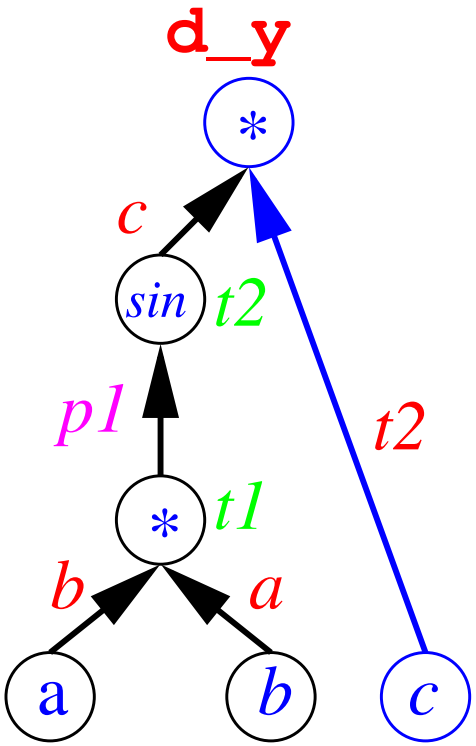

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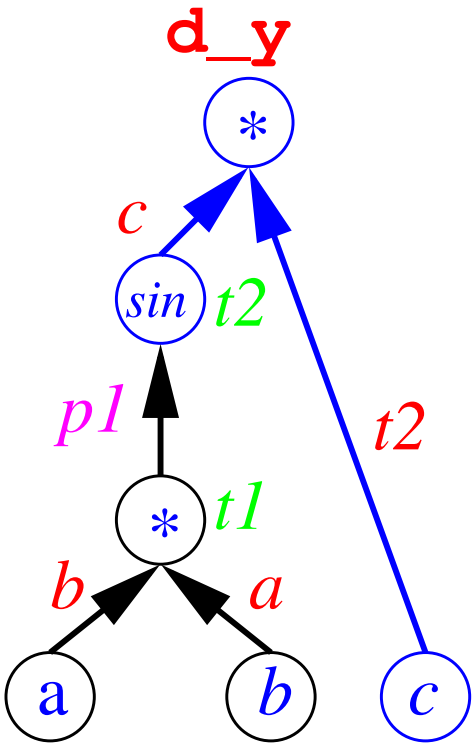

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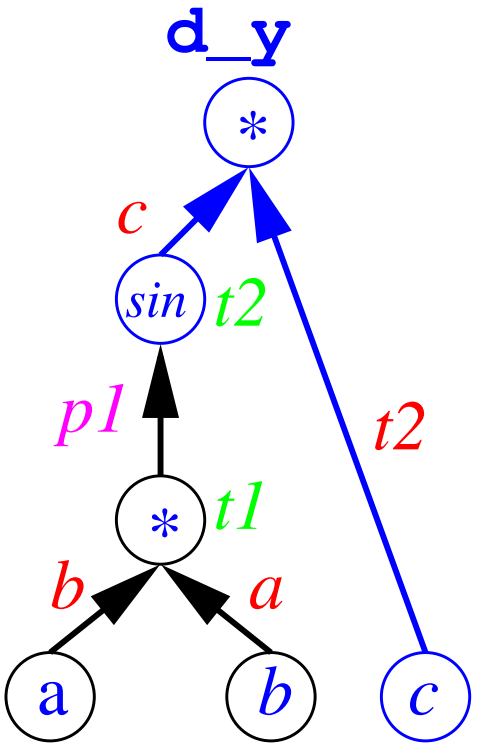

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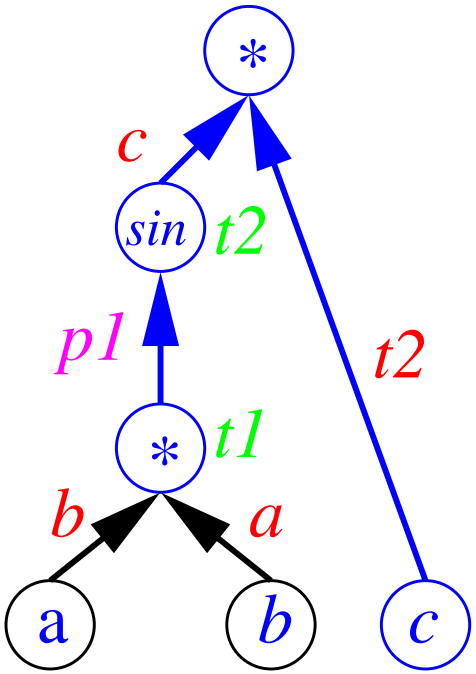

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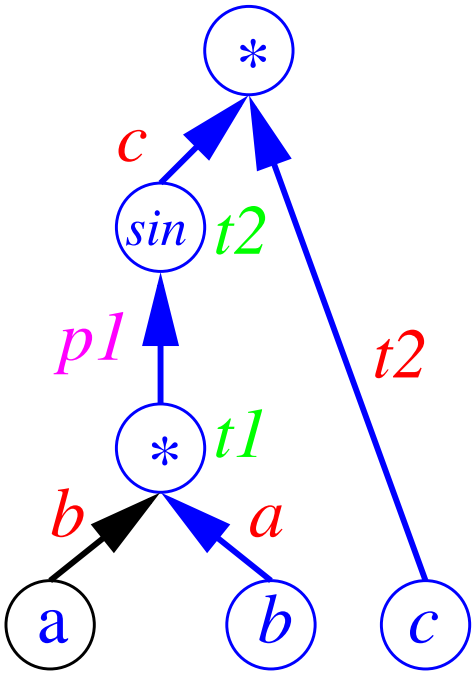

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d_t1 = p1*d_t2
d_b = a*d_t1
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- take a point (a_0, b_0, c_0), compute y, pick a weight $\bar{y}$
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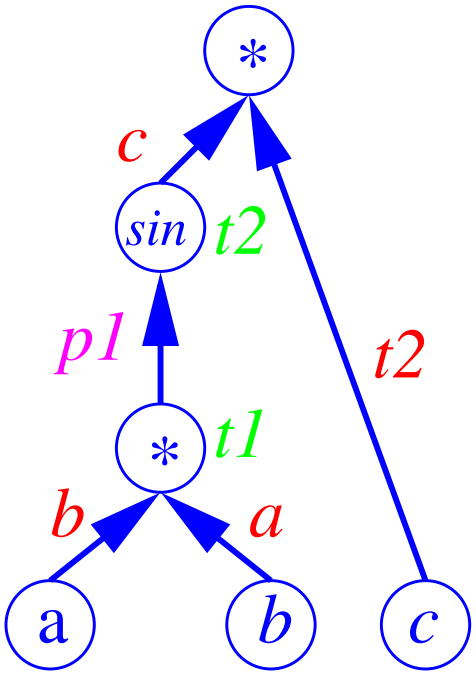
  $\bar{w} += \frac{\partial \phi}{\partial w} \; \bar{v}; \quad \bar{u} += \frac{\partial \phi}{\partial u} \; \bar{v}; \quad \bar{v} = 0$



backward propagation code appended:

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t1 = a*b
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d_c = t2*d_y
d_t2 = c*d_y
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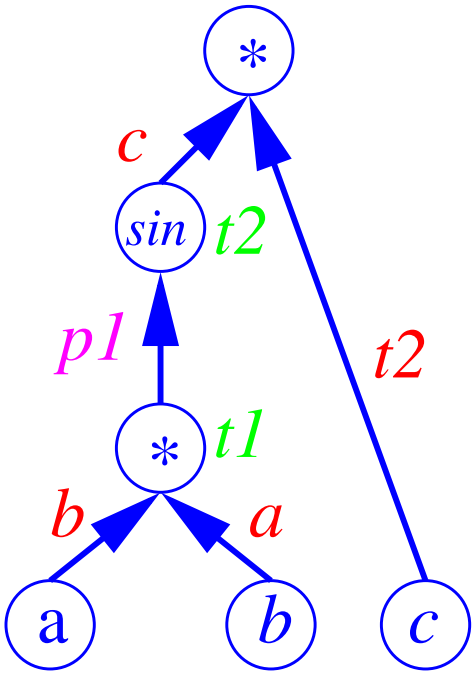

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What is in (d_a,d_b,d_c)?

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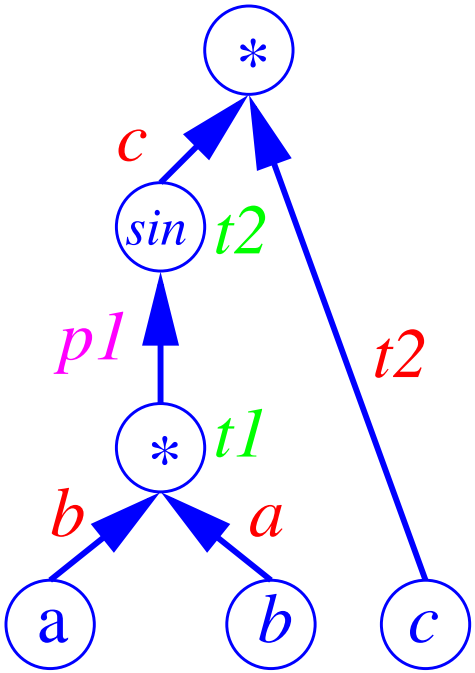
- $\bar{\boldsymbol{x}} = \bar{\boldsymbol{y}}^T \boldsymbol{J}$ computed at $\boldsymbol{x}_0$



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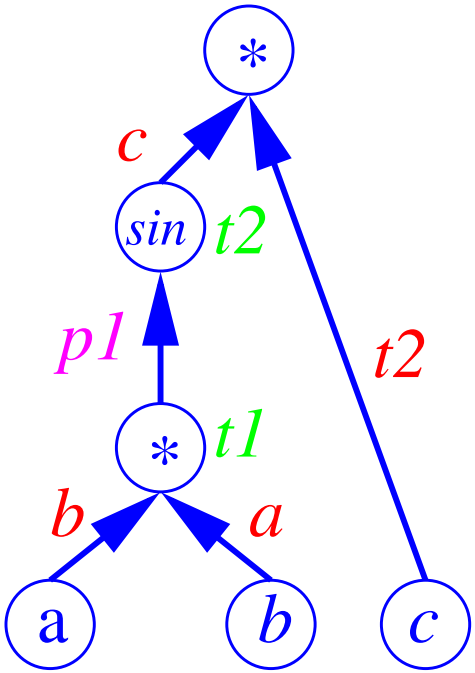

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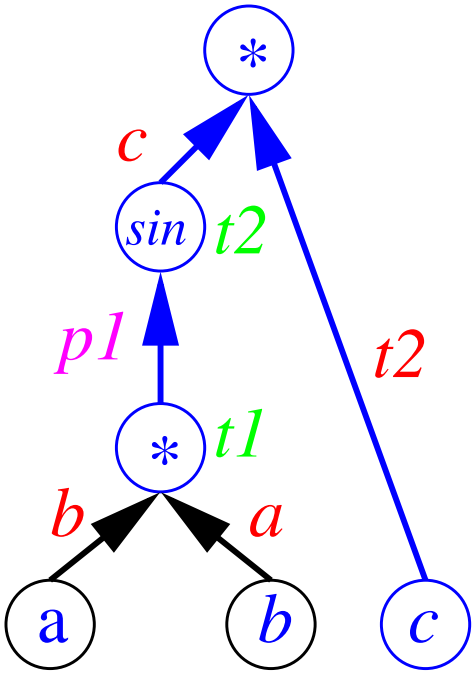

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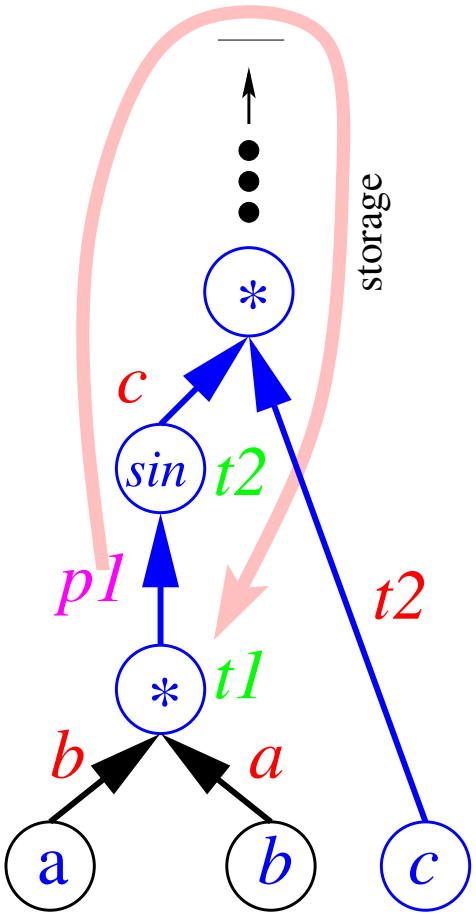

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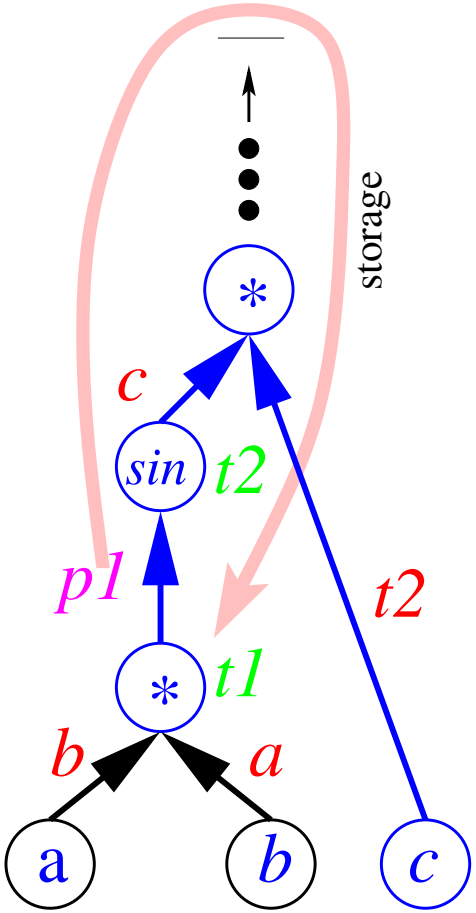

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Reverse mode with Adol-C.

Adol-C example

Adol-C: open source C++ operator-overloading library

Speelpenning example: $y = \prod_i x_i$ evaluated at $x_i = \frac{i+1}{i+2}$

```
 double *x = new  double[n];
 double  t = 1;
 double y;

for(i=0; i<n; i++) {
  x[i]   = (i+1.0)/(i+2.0);
  t *= x[i]; }
y = t;

delete[] x;
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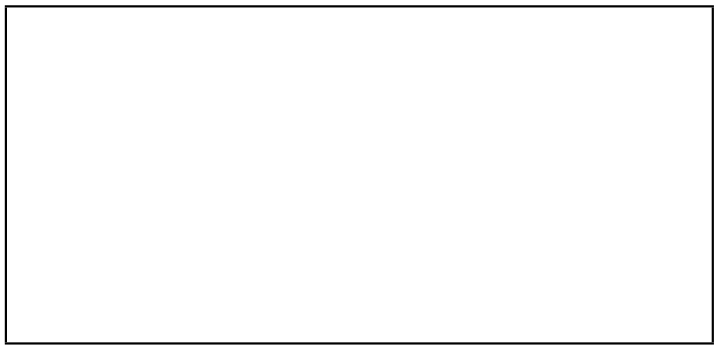

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 double y;
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t >>= y;
trace_off();
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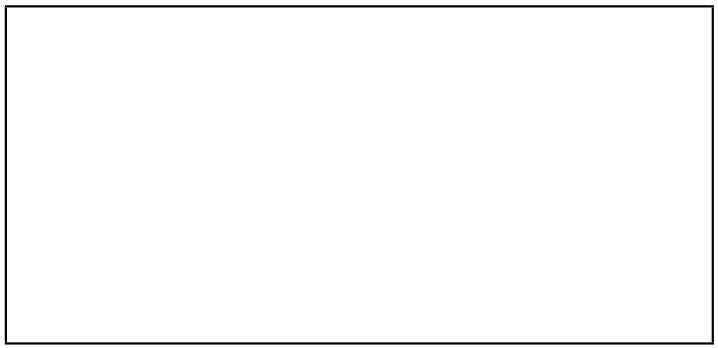

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use a driver :

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gradient(tag,
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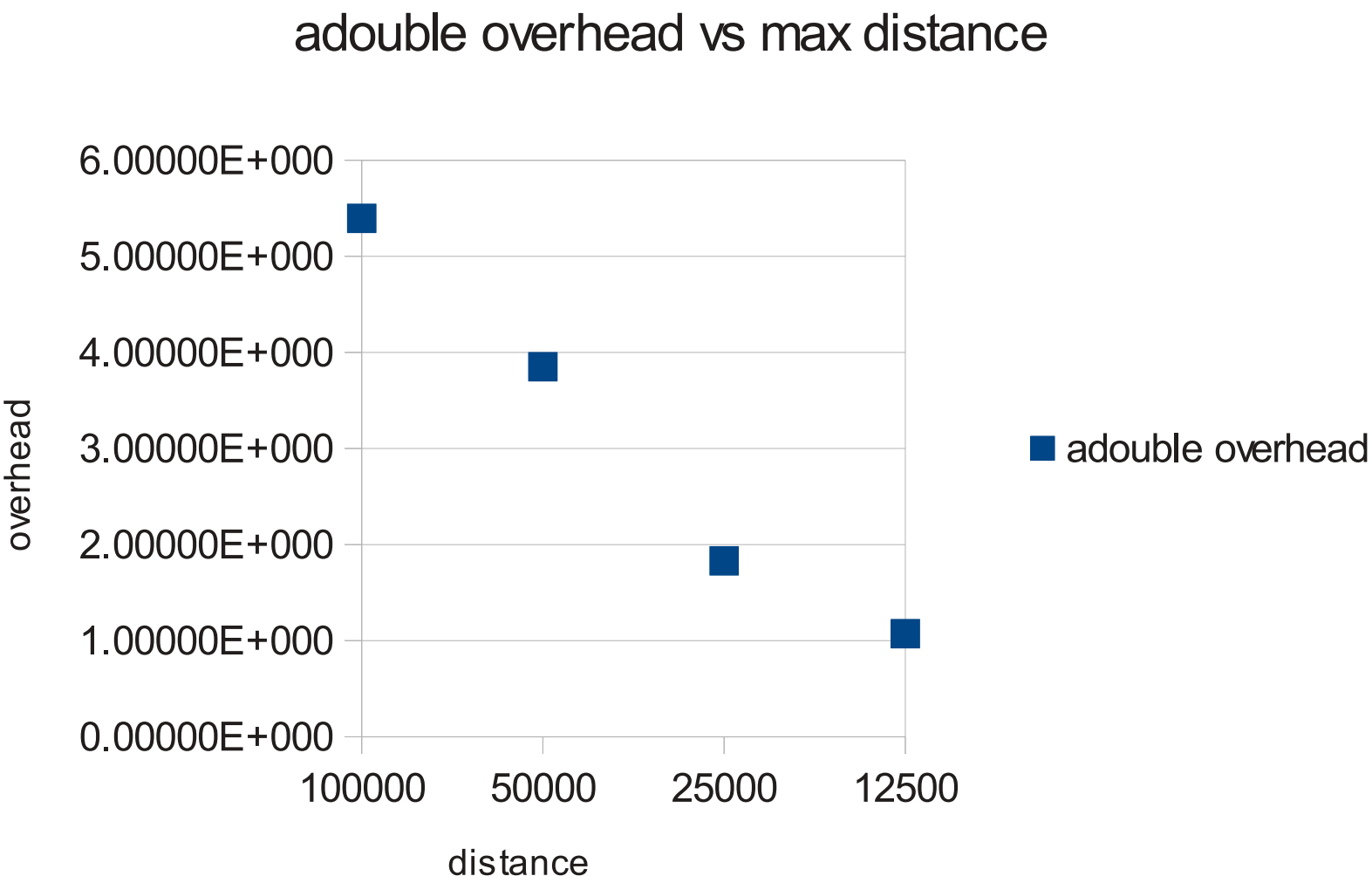

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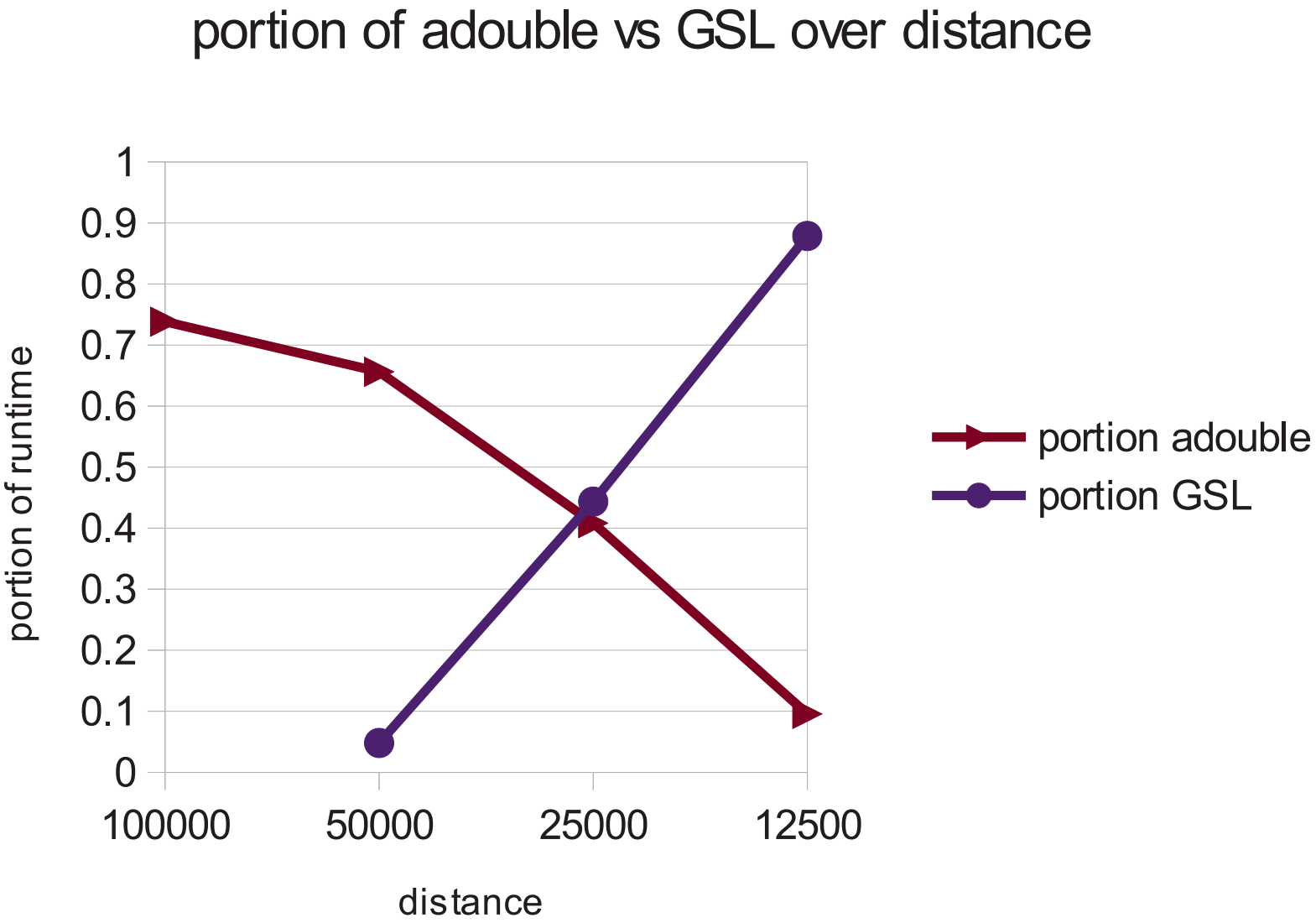

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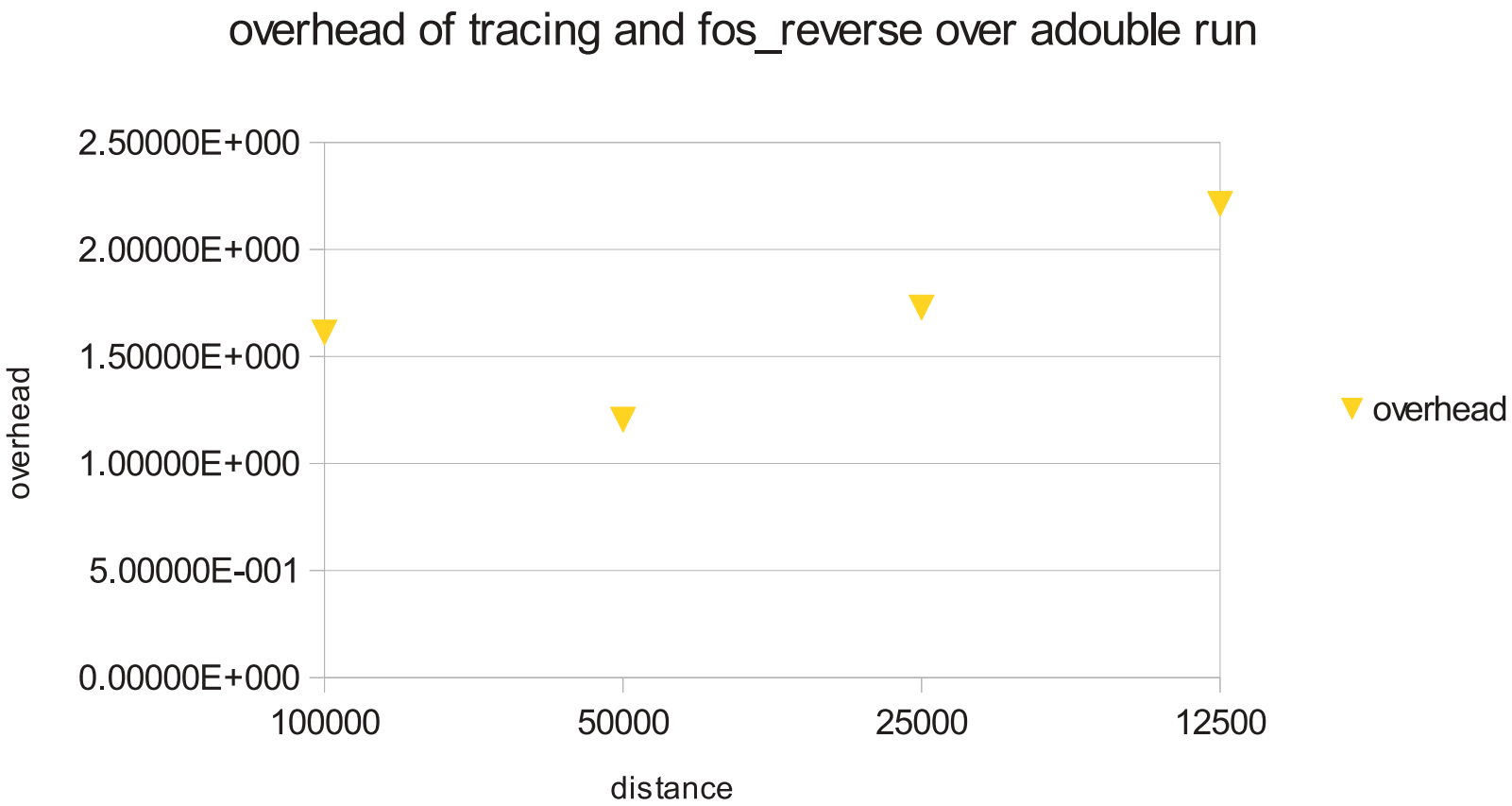

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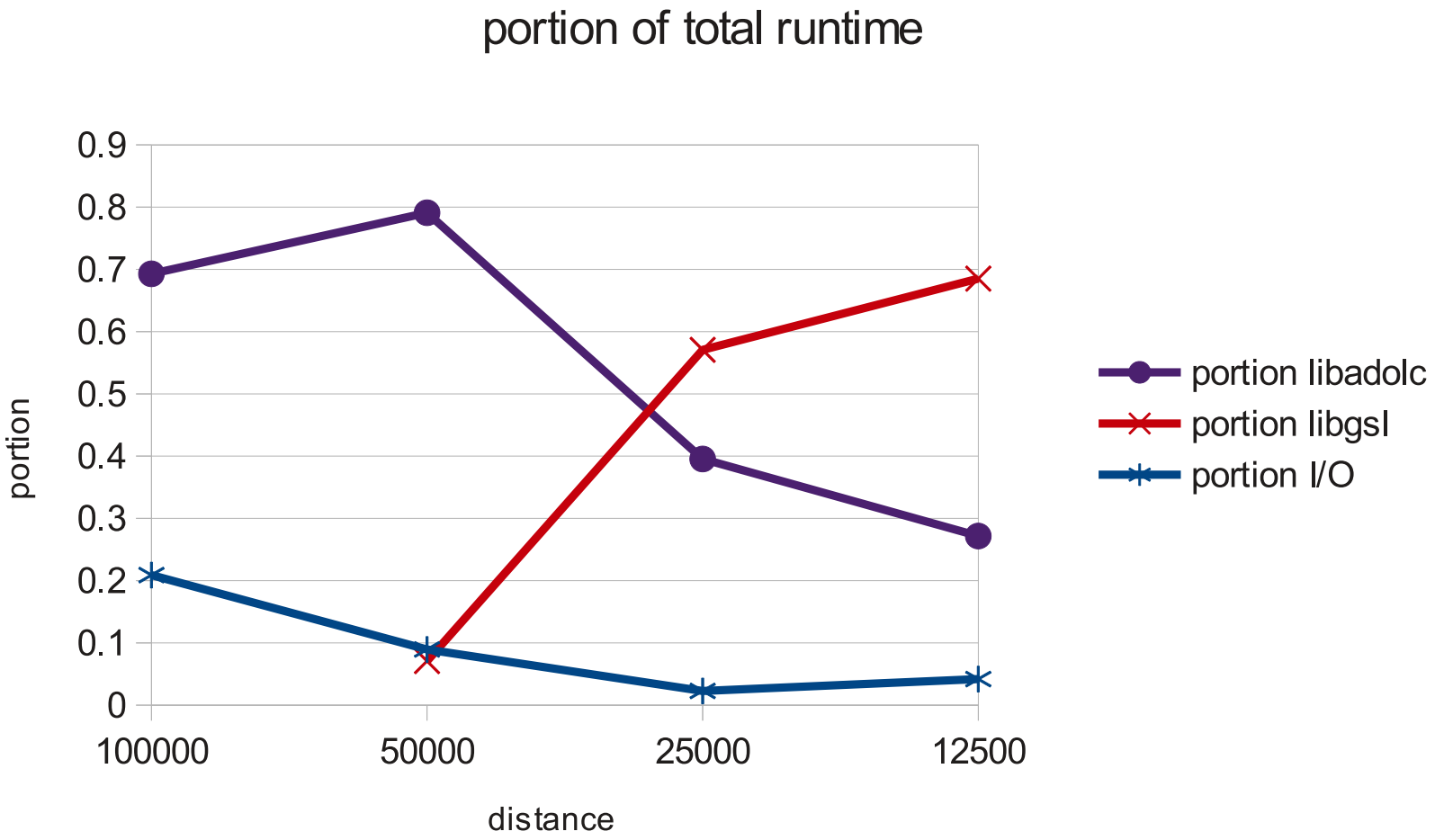

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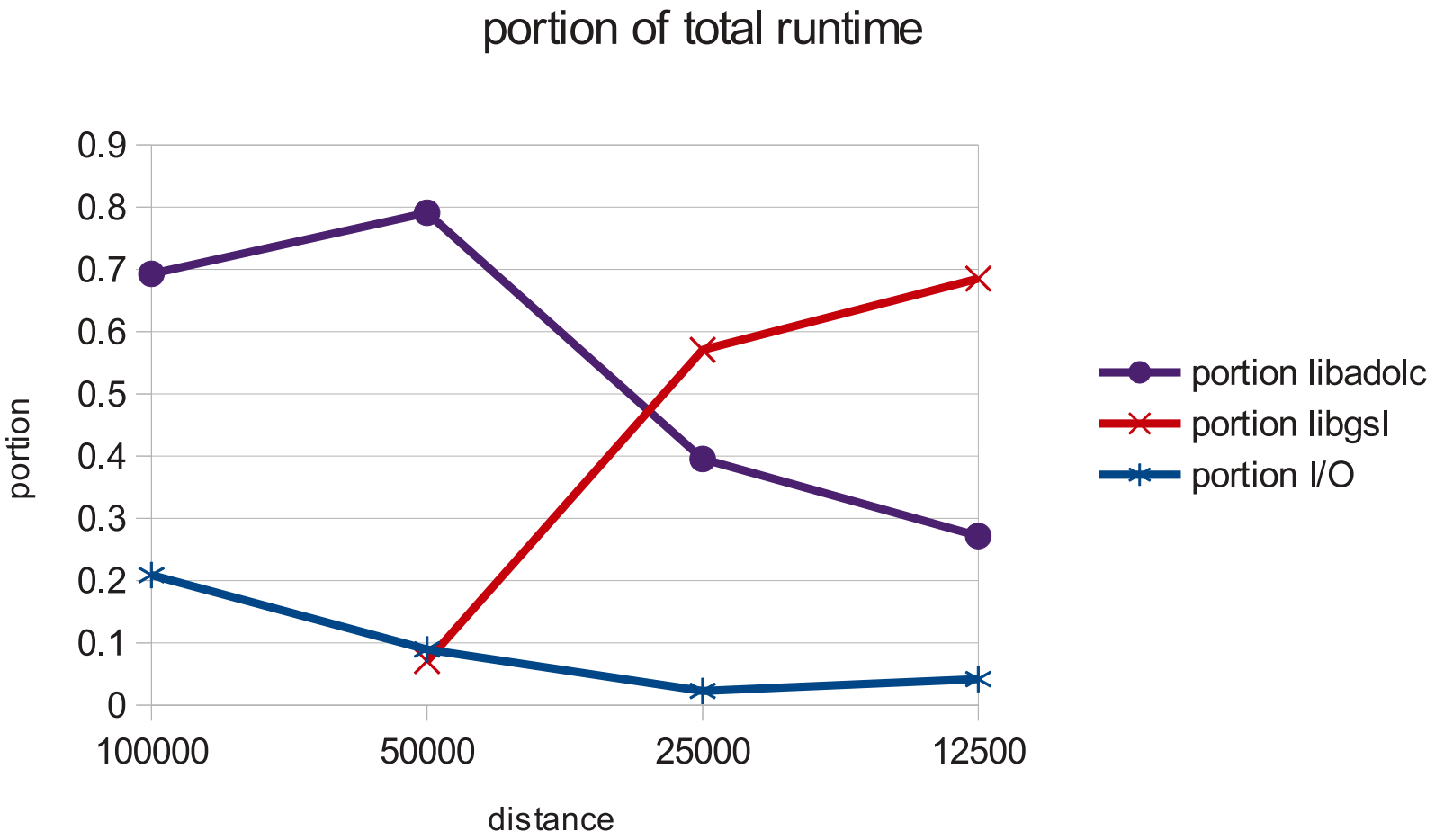
using "test3019" - an AD-enabled regression test



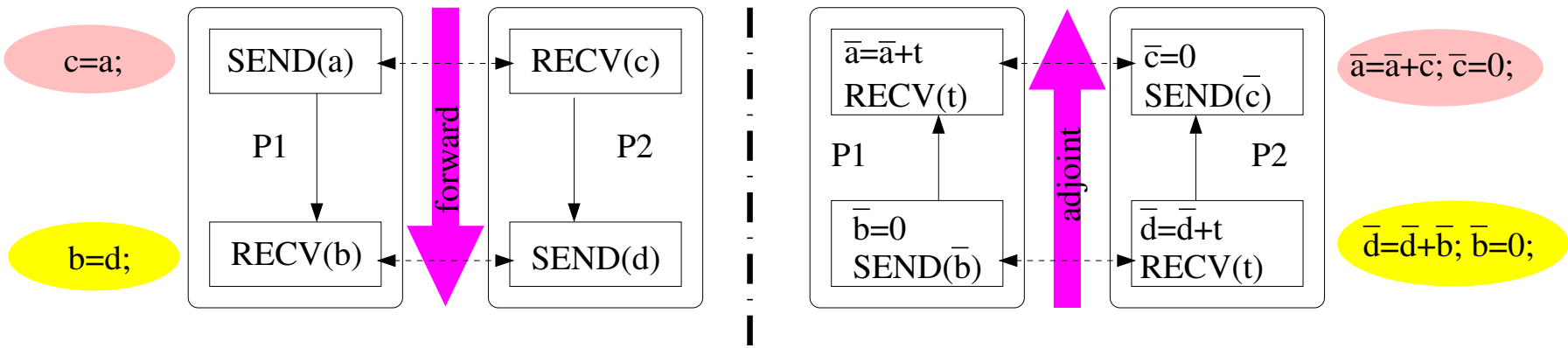
heavily skewed in Adol-C's advantage because of GSL

sidebar: Parallel with MPI (I)

- a simple MPI (pseudo) program with 6 calls :

```
mpi_init      // initialize the environment
mpi_comm_size // number of processes in the communicator
mpi_comm_rank // rank of this process in the communicator
mpi_send      // send (blocking)
mpi_recv      // receive (blocking)
mpi_finalize  // cleanup
```

- example reverse mode for blocking communication between 2 ranks and interpret as assignments



- use the communication graph as model

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- MPI emulator uses `memcpy` or `adouble` assignments resp.
- layer encapsulates all MPI switching $\Longrightarrow$ cleaner code

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- Adol-C has:
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  - (ii) typed, 4-way stack (tape+Taylors)

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- requires contiguous locations $\Longrightarrow$ enforced in `xNew` spec.

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- correspondence required the same way as in standard MPI
- practical problems with collectives distributed in the code proved it is easy to get wrong

Adjoinable MPI in Adol-C and ISSM (2)

template the MPI logic with 2 parameters like this pattern

```
1  #include <iostream>
2  typedef int DataType;
3  class TypeInfo {
4  public:
5    static DataType ourDoubleType;
6    static DataType ourIntType;
7  };
8  DataType TypeInfo::ourDoubleType;
9  DataType TypeInfo::ourIntType;
10
11 template <class T, DataType *typeOfT_p> class C {
12 public:
13   C(){};
14   ~C(){};
15   void foo(T aT) { std::cout << aT << " of type " << *typeOfT_p << std::endl; }
16 };
17
18 int main (void) {
19   TypeInfo::ourDoubleType=1;
20   TypeInfo::ourIntType=2;
21   C<double,&TypeInfo::ourDoubleType>().foo(2.0);
22   C<int,&TypeInfo::ourIntType>().foo(-1);
23   return 0;
24 }
```

not completed (yet) in ISSM

wrapping MUMPS

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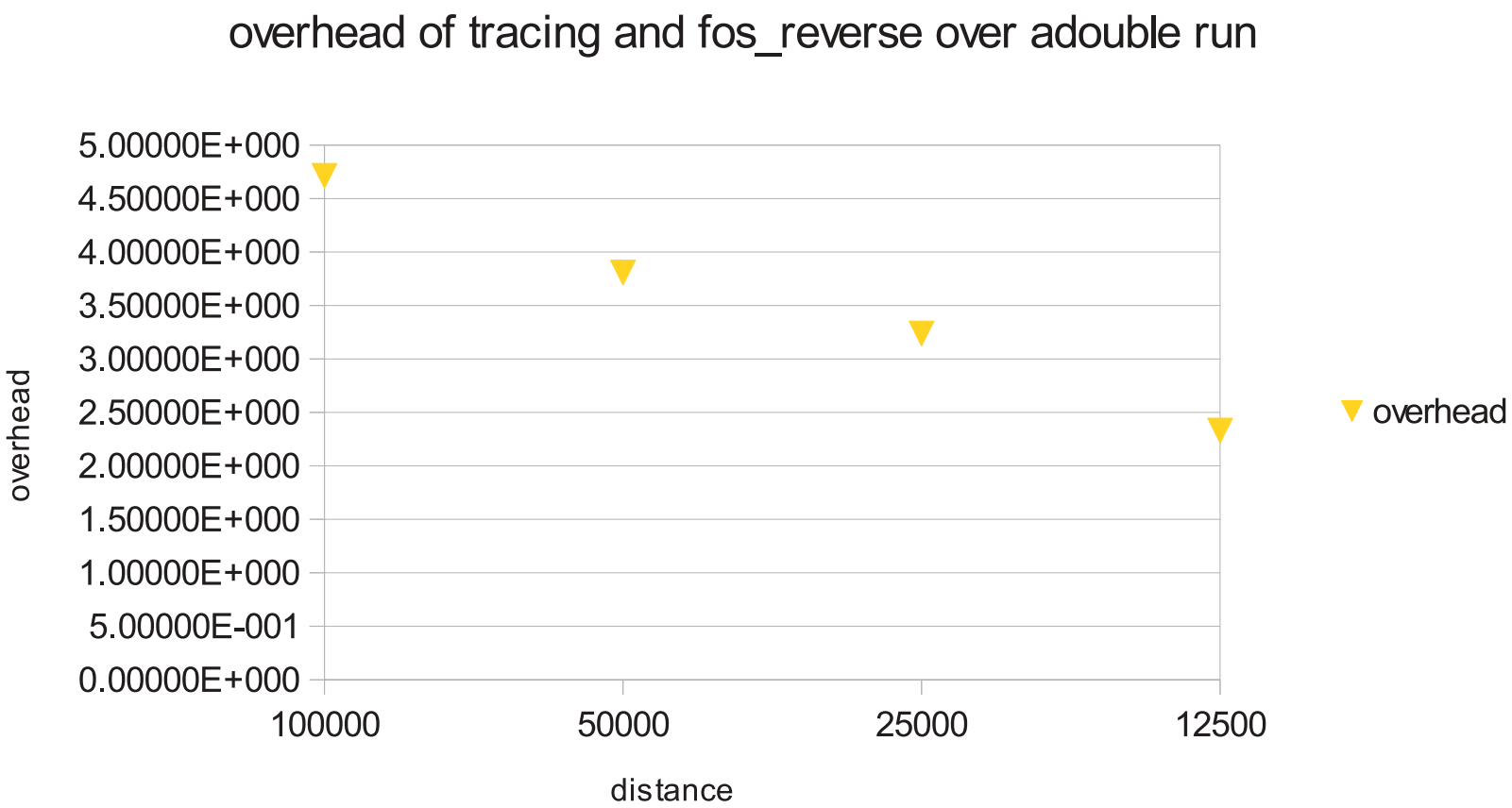
- revisit performance (by now $>$ 500 svn changesets later)

AdolC-ified ISSM performance - tracing & reverse (1)

test3019 - with contiguous locations, 3-way parallel MUMPS



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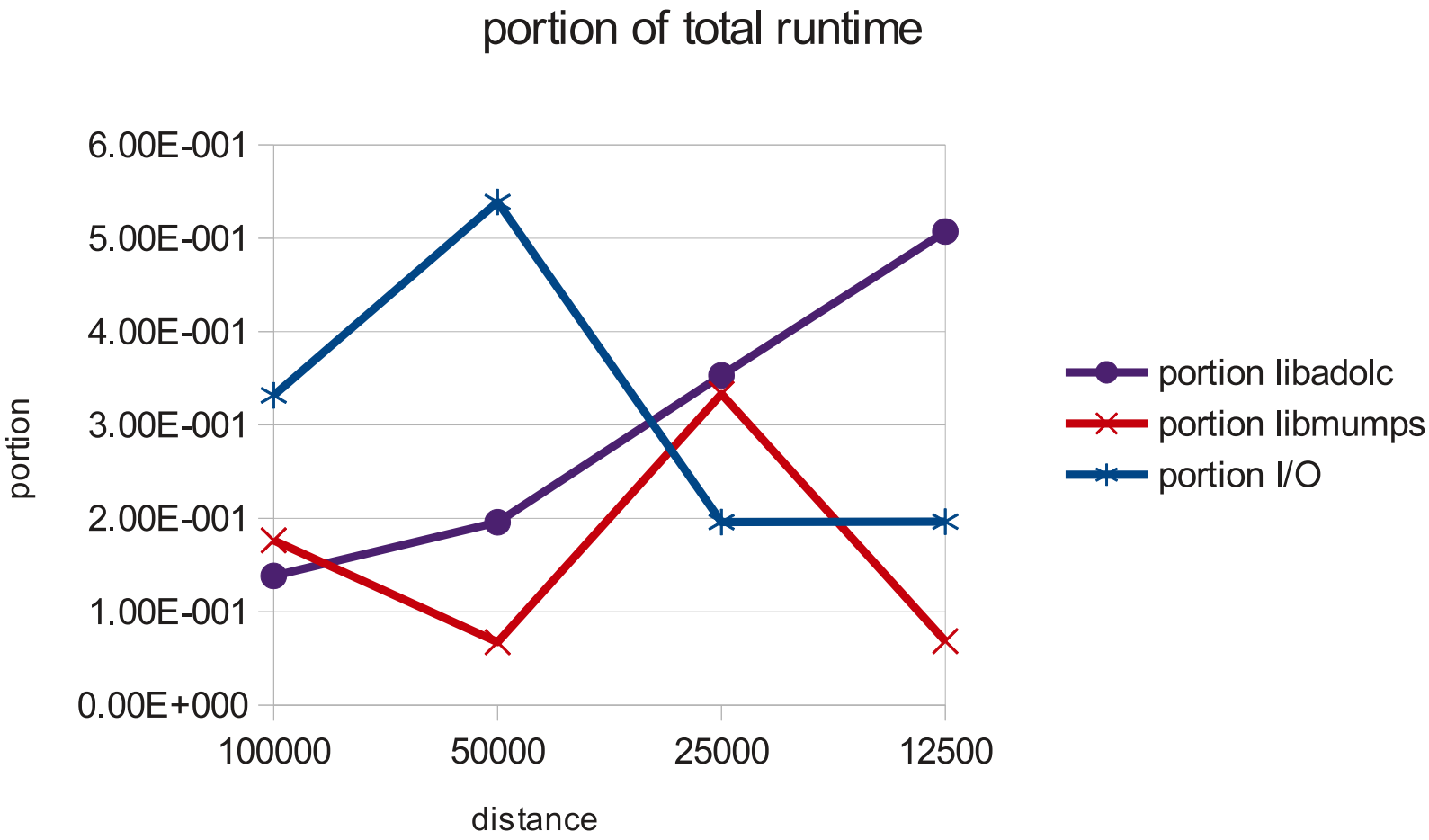

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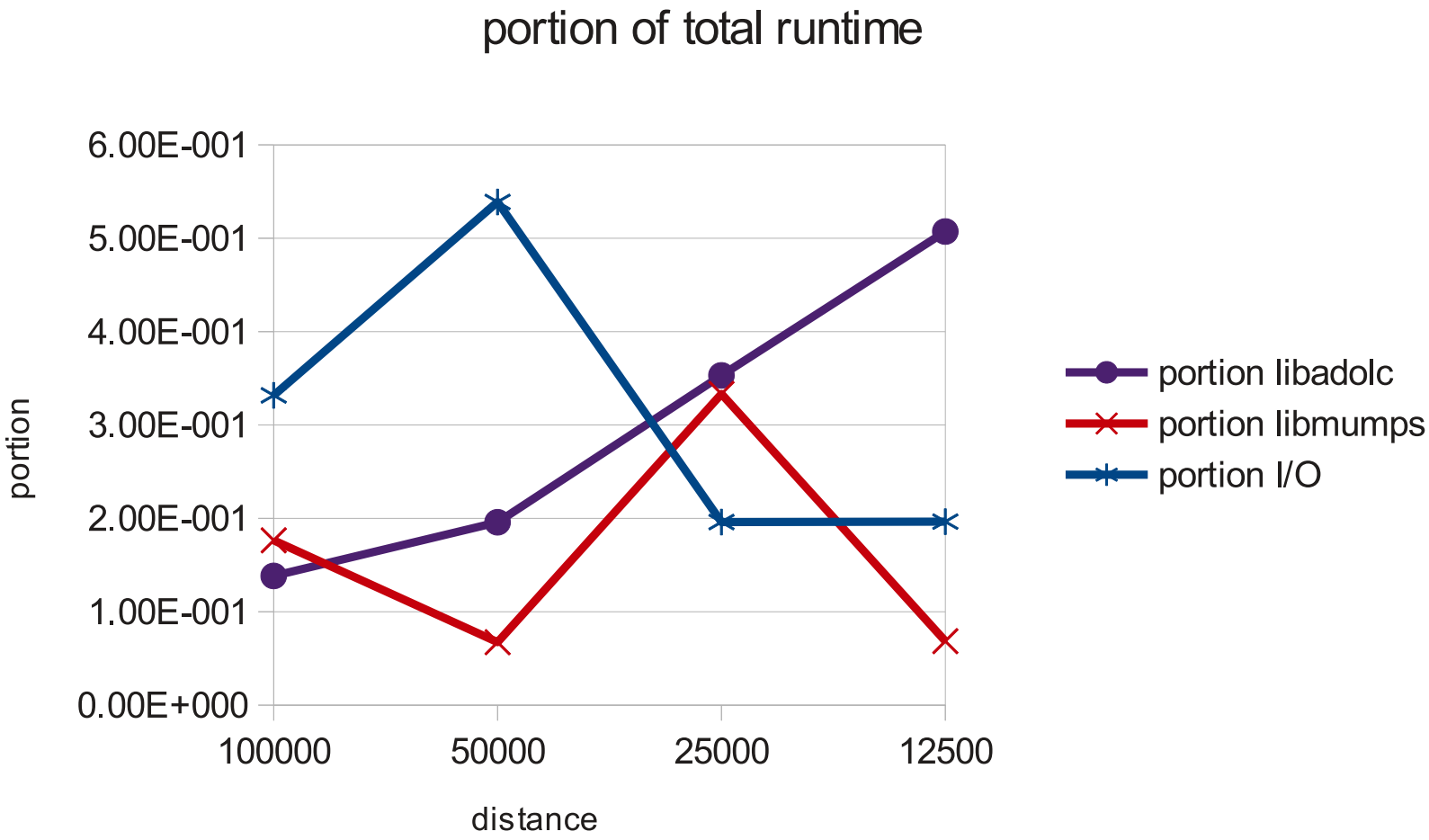

MUMPS is fast - more realistic picture

AdolC-ified ISSM performance - tracing & reverse (3)

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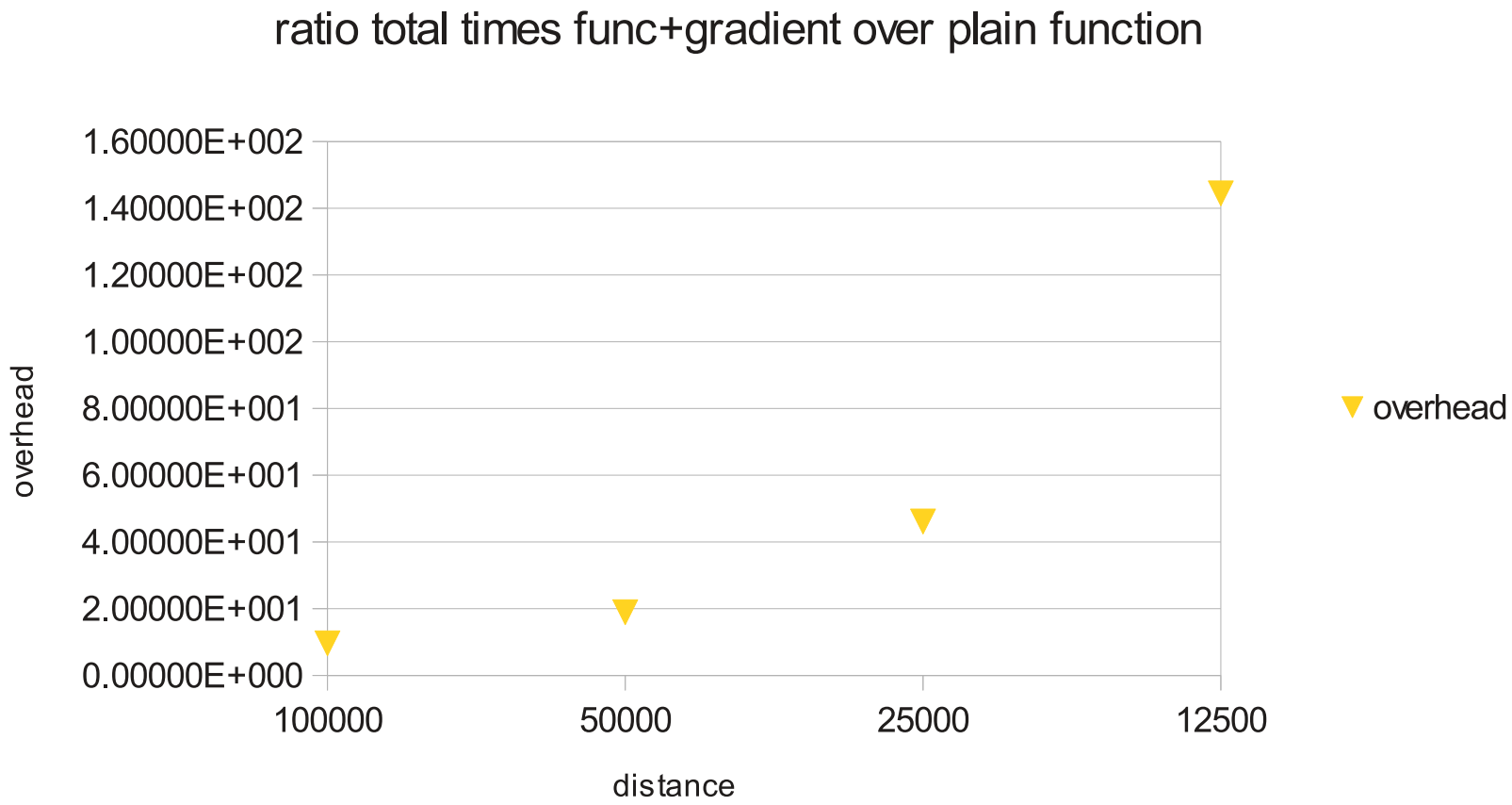

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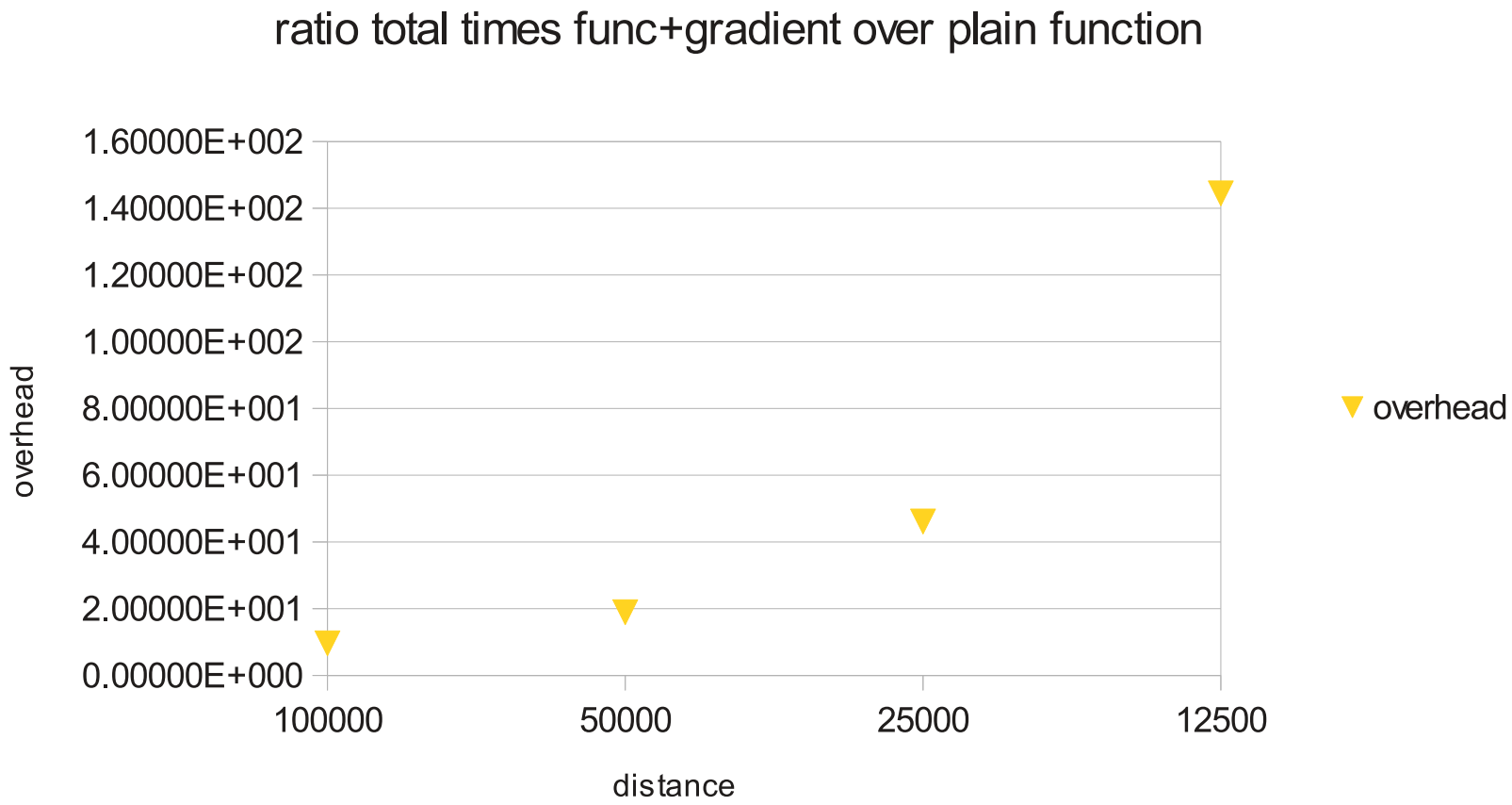

i.e. pretty nasty ... BUT

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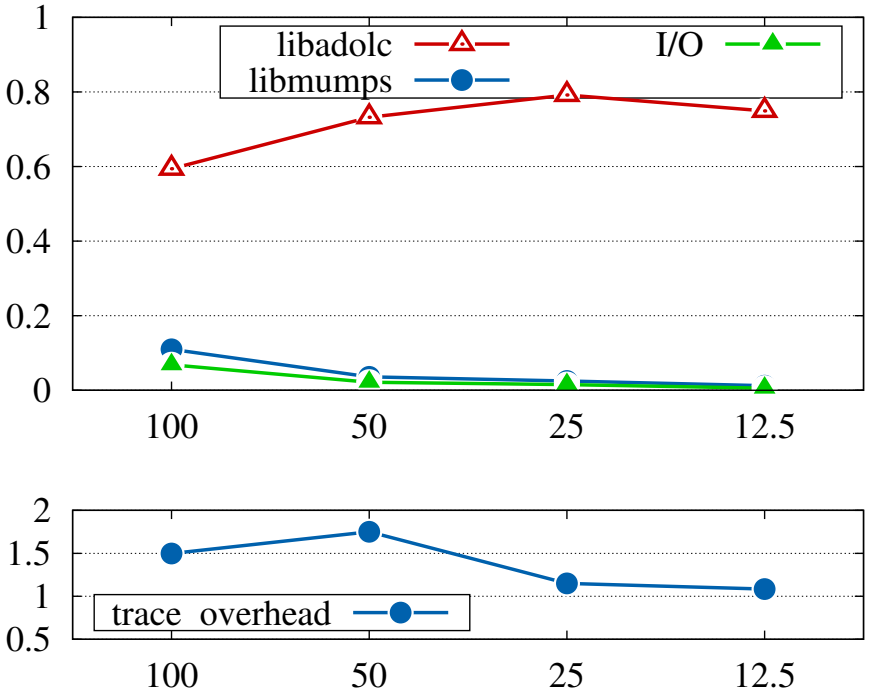
new 3-way parallel MUMPS



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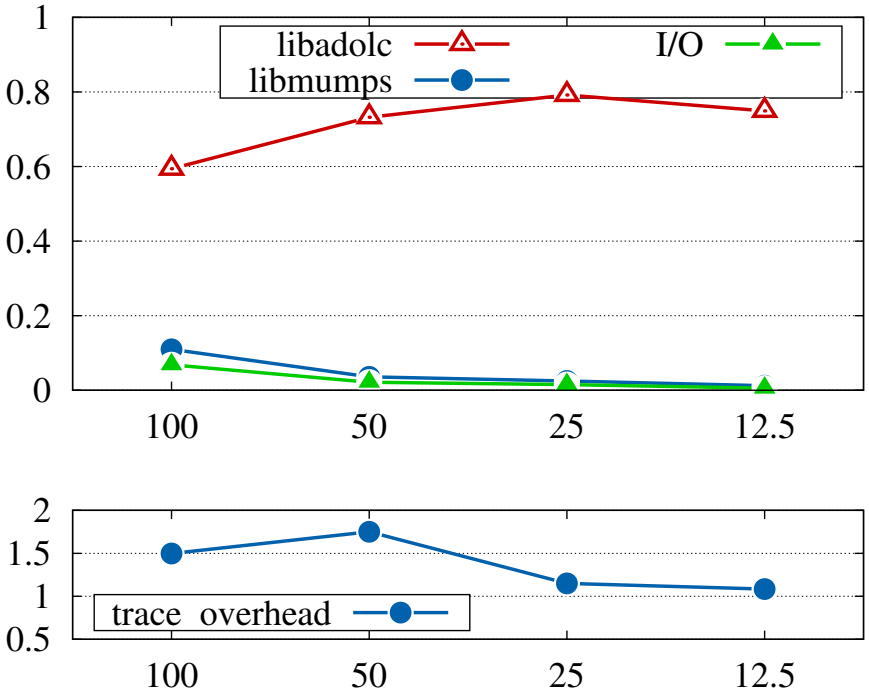

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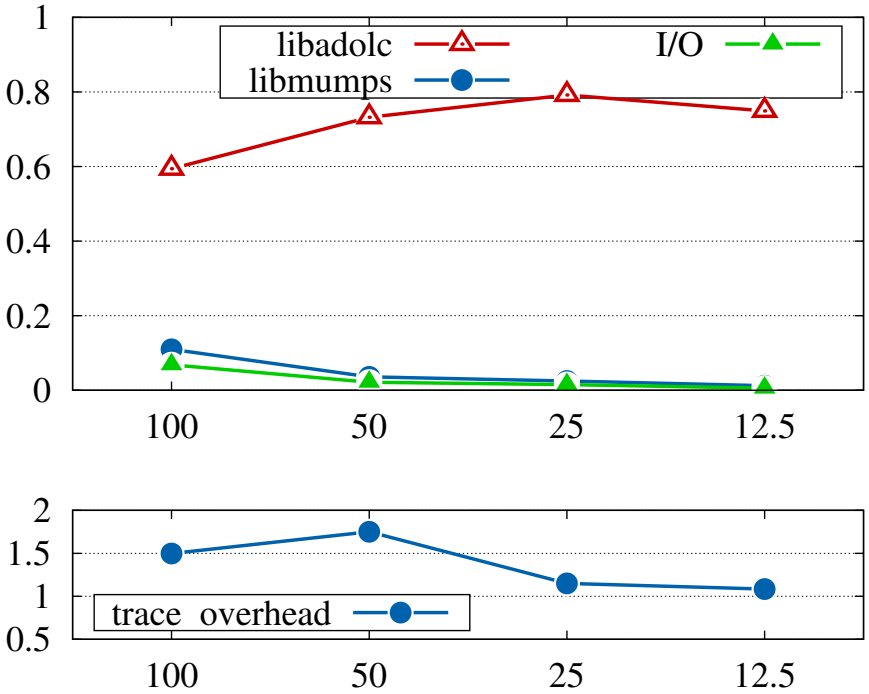

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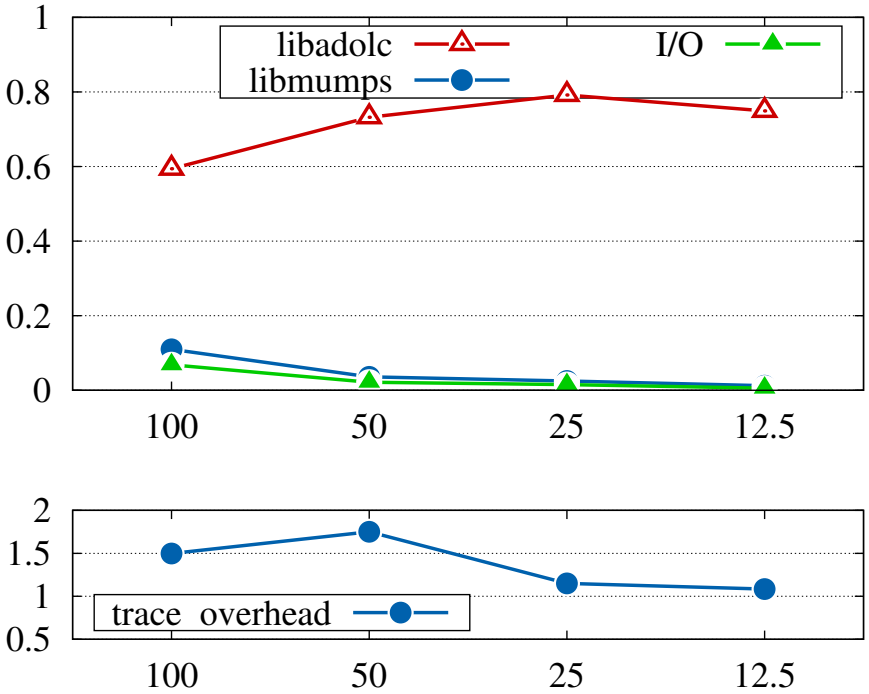

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- reflects theoretical result for reverse interpretation
- practically viable on Pleiades

AdolC-ified ISSM performance - outlook

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